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A Coupled Thermochemistry-Interior Ballistic Model and Application to Electrothermal-Chemical (ETC) Guns

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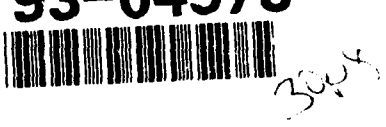

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In order to provide a more accurate description of the state of the propelling gas in electrothermal-chemical (ETC) gun simulations, the equilibrium thermochemical code BLAKE has been directly linked to a lumped parameter interior ballistics (IB) model and an inverse model. The inverse model utilizes experimental measurements of pressure, projectile position, and electrical energy input to infer the mass of propellant consumed at a timestep. In the linked models, computed value of the space-mean pressure is supplied directly to the codes, obviating the need for impetus and the ratio of specific heats in the calculation of energy. The linked thermochemistry-IB models are discussed and applied to experimental ETC data.

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TABLE OF CONTENTS

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LIST OF FIGURES

LIST OF TABLES

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1. INTRODUCTION

The electrothermal-chemical (ETC) gun, generically shown in Figure 1, is a propulsion concept which utilizes a low-mass, high-energy plasma to initiate and, hopefully, control the combustion/vaporization of the working fluid (propellant) during the ballistic cycle. Controlling combustion (exothermic working fluid) or vaporization (endothermic working fluid) of the working fluid in the ETC gun is necessary in order to tailor the pressure-time profile in the gun. Theoretically, tailoring the pressure-time profile to obtain a "flatter" and extended pressure curve should result in enhanced performance (increased muzzle energy) and provide a "softer" launch environment to enhance projectile integrity, especially for "smart" projectiles. In addition, precise control of the pressure history should also allow for the required projectile velocity repeatability required of indirect fire support (artillery) applications. An essential facet of understanding the control of the process through the plasma-propellant interaction is an accurate description of the energy release rate (J/s).

In previous work (Wren and Oberle 1990, 1992), the authors derived and implemented an inverse analysis of experimental ETC gun firing data to determine if a relationship between electrical energy input and energy release rates was indicated. For that analysis, variable thermochemical properties of the propellant gas/plasma mixture were assumed to be dependent only on the constitutive components of the propellant and the electrical energy density (kJ/g; ratio of total electrical energy input to consumed propellant). Implementation of this variable thermochemistry in the computer model was through the use of "look-up" tables, similar to Table 1 for JA2 propellant (Bunte and Oberle 1989). Values in the tables were obtained using the thermodynamic equilibrium code BLAKE (Freedman 1982) at a fixed loading density *(ld)* (g/cm^3; ratio of consumed propellant to free volume) of 0.2 g/cm^3.

However, a detailed analysis of the results from the study identified several potential shortcomings related to the use of look-up tables for the thermochemical properties. First, the values of the thermochemical properties are dependent on the loading density, as illustrated in Table 2 for JA2 propellant.

Fortunately, it has been shown (Robbins 1991) that for traditional solid propellant modeling, consideration of the loading density dependence of values of the thermochemical properties has no significant (<1%) impact on simulation results, even through loading density (ratio of mass of gas to gas volume in g/cm^3) can vary over a large range, as illustrated in Figure 2. Similar results have yet to be demonstrated for ETC simulations. In fact, for the ETC gun, the problem of determining the energy

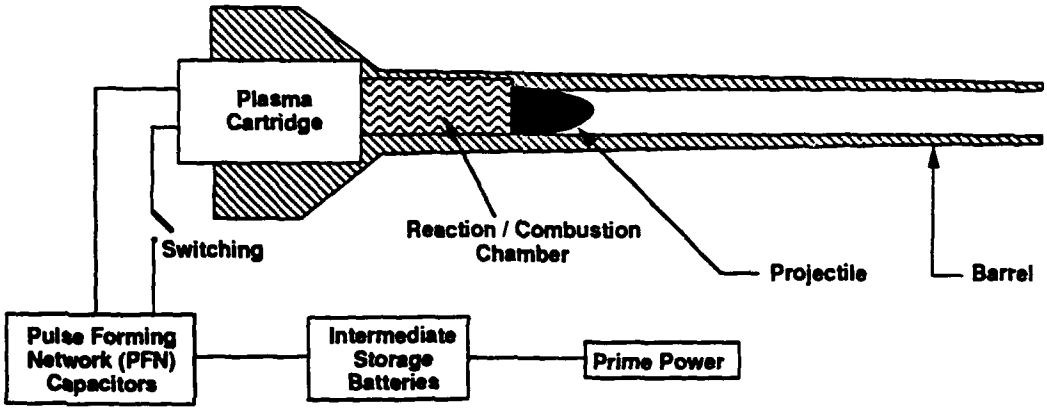


Figure 1. Schematic of ETC gun.

Table 1. Variable Thermochemical Properties for JA2 as a Function of Electrical Energy Density

Electrical Energy Input (kJ/g)	Temperature (K)	Impetus (J/g)	Molecular Weight	γ	Specific Energy (J/g)
0	3,424	1,144	24.886	1.2254	5,075
1	3,959	1,334	24.686	1.2219	6,012
2	4,401	1,504	24.337	1.2219	6,778
3	4,776	1,663	23.882	1.2241	7,421
4	5,113	1,819	23.378	1.2275	7,996
5	5,429	1,975	22.857	1.2316	8,528

Table 2. Loading Density Dependence of Values for Thermochemical Properties Computed by BLAKE for JA2 Propellant

Loading Density (g/cm^3)	Temp (K)	Impetus (J/g)	Molecular Weight Gas	Co-Vol (cm^3/g)	Frozen γ	Specific Energy (J/g)
0.1000	3,371	1,134.5	24.704	1.031	1.2229	5,090
0.2000	3,395	1,140.4	24.749	0.991	1.2254	5,059
0.3000	3,408	1,143.7	24.664	0.948	1.2305	4,962
0.4000	3,417	1,145.8	24.797	0.903	1.2379	4,816
0.5000	3,425	1,147.3	24.820	0.858	1.2474	4,367
0.6000	3,431	1,148.3	24.846	0.814	1.2589	4,435

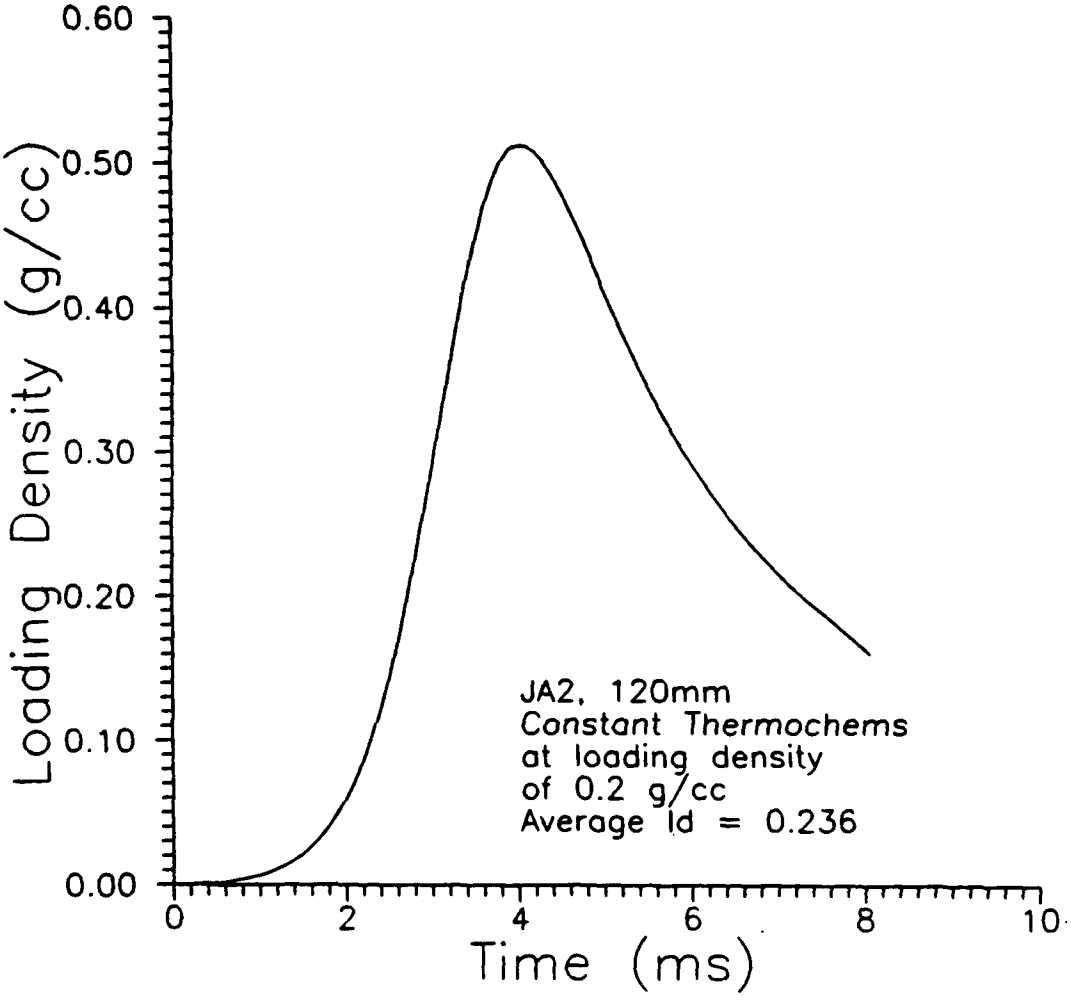


Figure 2. Loading density history in a 120-mm simulation using IBHVG2 (Anderson and Fickie 1987).

release rate is further complicated by the staged introduction of electrical energy which produces combustion gases with even larger changes in thermochemical values compared to solid propellants alone (see Tables 1 and 2). Thus, it appears that for ETC interior ballistic (IB) calculations, both the loading and electrical energy densities should be considered in determining the energy release rate. Although some earlier (Oberle 1989; Gough 1989; Wren and Oberle 1990, 1992) investigations of ETC performance considered variations in thermochemical values (energy release rate) as a function of electrical energy density, no work has incorporated both variations in loading density and electrical energy density.

A second and potentially more serious shortcoming to the use of a look-up table is the accuracy of the table values as the electrical energy density increases to produce average gas temperatures above 5,000 K. The thermochemical values typically utilized in IB codes are flame temperature, chemical energy, and covolume based on polynomial fits to experimental values of specific heat at constant pressure, C_p. In the case of BLAKE, the JANAF data for C_p for all of the product gases are computed using statistical mechanics based on spectroscopic data. Although these calculations can be readily extended well above 5,000 K, tables of these data traditionally terminate around 5,000 K. Thus, the fittings of the data are valid only to 5,000 K. The polynomial fitting functions for C_p take on values to plus or minus infinity outside the fitting range; C_v will behave similarly. Their ratio γ will approach one in the limit, and the value of γ above 5,000 K is thus useless for the ETC application (Freedman 1991), since gas temperatures for ETC propellants may be high, at least locally, where the plasma temperature is typically in the range of 10,000–15,000 K. Thermochemical values for high electrical energy densities, and hence, high temperatures, are thus ill-defined and based on extrapolated polynomial fits.

Traditionally, the chemical energy is determined primarily from impetus and the ratio of specific heats (γ). Since γ is directly related to specific heat at constant pressure and C_p is supplied to BLAKE as experimental data, it might be expected that extrapolated values of γ are particularly poorly behaved. In the previous effort (Wren and Oberle 1990, 1992) to determine energy release rates, an adequate description of γ above 5,000 K was a major shortfall. In addition, the γ calculated by BLAKE is for the gas phase only and does not address the use of solid particles used in some experimental ETC propellants. Previous IB calculations have shown that traditional measures of "goodness" of the propellant may not be applicable to ETC propellants containing large amounts of solid particles such as aluminum (White and Oberle 1989).

Therefore, to address the question as to whether fixed thermochemistry will be sufficient to describe the ETC IB process and bypass the use of γ, the thermochemical code BLAKE has been directly linked to a lumped parameter IB model and an inverse model developed earlier. The computed value of the space-mean pressure is supplied directly to the IB and inverse codes, thereby directly including the effect of the loading density and electrical energy density and obviating the need for impetus and γ in the calculation of energy. Although the space-mean pressure is also related to the experimental values of specific heat at constant pressure, it is expected to be much more reliable since it is a function of several well-defined variables (Freedman 1991).

2. DESCRIPTION OF THE *MODELS*

The thermochemical code BLAKE was revised to serve as a subroutine to a main calling program. BLAKE requires the constituent data as well as values of electrical energy density (electrical energy input in kilojoules/mass of propellant consumed in grams) and loading density. The thermochemical code then returns the space-mean pressure of the gas assuming equilibrium thermodynamics.

Two implementations of the thermochemical code are explored in this report. The first is a traditional time-marching IB formulation using a Lagrange gradient and expressed in a form to utilize the space-mean pressure, denoted as IBBLAKE. This formulation uses as input the gun geometry, projectile mass and resistive pressure profile, propellant geometry, propellant thermochemistry, and electrical energy history. By iterating on the mass of propellant consumed in a time step, which is passed to BLAKE along with the electrical energy, the conservation equations are satisfied. Since the equilibrium state of the gas at any time step must consider the work during expansion in terms of projectile kinetic energy, fluid kinetic energy, and other losses (assumed 0.0 for the purposes of this study), the electrical energy is reduced by the predicted kinetic energies of the gas and projectile on any time step. (Note: This may result in a negative electrical energy input to the BLAKE calculation.) The mass of propellant consumed is then determined and the pressures, projectile motion, and other IB information are output.

Secondly, the BLAKE subroutine was integrated into an inverse code (Wren and Oberle 1990, 1992) which utilizes experimental data in order to infer the mass of propellant consumed at any time step. The linked model is denoted as INVBLAK. The inverse model uses as input experimental values of projectile position, electrical energy input to the gun, and chamber pressure. Assuming a Lagrange gradient, it is then possible to infer space-mean pressure in the experiment since the gas volume, projectile kinetic

energy, and fluid kinetic energy are known. The BLAKE subroutine is used to supply a space-mean pressure based on an electrical energy density and loading density for the propellant gases. By iterating on the mass of propellant consumed, the space-mean pressure in the experiment and the space-mean pressure predicted by BLAKE are simultaneously satisfied. The output is then the mass of propellant consumed at time step.

3. COMPARISON WITH SOLID PROPELLANT MODEL

In order to assess the effect of incorporating updated thermochemical values in a solid propellant only simulation, the gun described in Table 3 was modeled with IBHVG2 and IBBLAKE. To perform the simulation, a choice concerning the burn rate and, hence, the mass generation rate for the solid propellant, must be made. For both IB codes, the burn rate is provided in the form $r = bP^n$. If fixed thermochemical values are utilized in the IB code, then the choice for the burn rate is straightforward. Use the coefficient b and exponent n determined via closed chamber data and the fixed thermochemical values. (Note that the burn rate is thus a function of the thermochemical values). However, if variable thermochemical values are to be used in the IB code, then the burn rate should be adjusted to be consistent with the closed chamber data and thermochemical values. Since for this report the thermochemical values are a function of loading density, it was necessary to adjust the burn rate to account for the variability in ld shown in Figure 2. One approach would be to perform an extensive series of closed chamber firings at different loading densities. However, such a series of firings was not feasible for this report.

Table 3. Gun Parameters Used in Simulation

Bore Diameter: 120 mm Chamber Volume: 9,750 cm^3 Projectile Travel: 475 cm	Projectile Mass: 11.4 kg Charge Mass: 8.8 kg Propellant: JA2

Thus, the burn rate as a function of loading density is estimated by the following approach. The final equation for computing the burn rate r from closed chamber data is

$$r = \frac{\dot{m}}{\rho A}, \tag{1}$$

where $\dot{m}$ is the time rate of change of mass, ρ the material density, and A the reacting surface area. Assuming constant propellant density, ρ, and a neutral (constant) reacting surface area, A, the burn rate is directly proportional to the time rate of change of the mass, $\dot{m}$,

$$r = k\dot{m}. \tag{2}$$

Now the mass history (mass vs. time) is determined from the closed chamber pressure history by determining the total chemical energy necessary to produce the observed pressure and the relation,

total chemical energy *(TCE)* = mass propellant consumed * propellant specific energy

$$= m * e\,. \tag{3}$$

If variable thermochemical values are utilized, then the propellant specific energy, e, will also be a function of loading density. However, the total chemical energy required is dependent only on the observed closed chamber pressure.

Thus,

$$m_{ld1}(P_1) * e_{ld1}(P_1) = TCE(P_1) = m_{ld2}(P_1) * e_{ld2}(P_1)\,, \tag{4}$$

where P_1 represents an observed pressure, and *ld*1 and *ld*2 values are associated with two different loading densities. To compute $\dot{m}$, consider two pressures, P_1 and P_2, measured in a time step Δt. From Equation 4,

$$\frac{m_{ld1}(P_2)\,e_{ld1}(P_2) - m_{ld1}(P_1)\,e_{ld1}(P_1)}{\Delta t} = \frac{m_{ld2}(P_2)\,e_{ld2}(P_2) - m_{ld2}(P_1)\,e_{ld2}(P_2)}{\Delta t}\,. \tag{5}$$

However, the specific energy is a function of loading density, not pressure; thus,

$$\dot{m}_{ld1}\, e_{ld1} = \dot{m}_{ld2}\, e_{ld2} \tag{6}$$

or

$$\frac{\dot{m}_{ld1}}{\dot{m}_{ld2}} = \frac{e_{ld2}}{e_{ld1}} . \tag{7}$$

Combining Equations 2 and 7,

$$\frac{r_{ld1}}{r_{ld2}} = \frac{k\dot{m}_{ld1}}{k\dot{m}_{ld2}} = \frac{e_{ld2}}{e_{ld1}} \tag{8}$$

or

$$\frac{r_{ld1}}{r(ld = 0.2 g/cm^3)} = \frac{e_{ld1}}{e(ld = 0.2 g/cm^3)} , \tag{9}$$

assuming that the closed chamber data has been fitted with a one-part burn rate, which is usually the case. Equation 9 is used to adjust the burn rate as a function of loading density. For the single-perforated grain under consideration, the neutral surface area assumption is felt to be reasonable.

The results are shown in Table 4. It can be seen that the results are in good agreement, indicating that the approximation of the thermochemistry of the propelling gas using constant thermochemical values at a *ld* of 0.2 g/cm^3 and a pressure-dependent burn rate law based on a *ld* of 0.2 g/cm^3 used in IBHVG2 are reasonable. Thus, it appears that constant thermochemical values at a *ld* of 0.2 g/cm^3 provides a good simulation of solid propellant performance.

Table 4. Comparison of IBHVG2 and IBBLAKE for Simulation of 120-mm Gun Using Single-Perforated JA2 Propellant

	Maximum Pressure (MPa)	Muzzle Velocity (m/s)
IBHVG2	572	1,403
IBBLAKE	570	1,415

In the case of ETC propellants, energy is not only a function of loading density but a function of electrical energy density as well. Figure 3 shows a graph of energy vs. *ld* vs. electrical energy density for a representative candidate ETC propellant of 80% by mass of HAN and methanol in a stoichiometric mixture and 20% water. Current lumped parameter ETC IB models using variable thermochemistry utilize tables of energy vs. electrical energy density at a constant *ld* of 0.2 g/cm^3. Figure 3 shows significant variation of energy of up to 30% at a constant $ld = 0.2$ g/cm^3, with electrical energy densities in the range of 0.4 kJ/g to 2.0 kJ/g. Thus, it might be expected that greater differences between IBHVG2 and IBBLAKE would be observed.

In order to determine a qualitative difference between the two types of simulations (and since a burning rate is not known for the ETC propellant considered), the simulation is performed with all input parameters identical to those used previously for the solid propellant except that the thermochemical properties are changed to those of the HAN, methanol, and water mixture and the burning rate is not adjusted. A comparison of the maximum pressure and muzzle velocity is shown in Table 5. The maximum breech pressures are comparable, and the projectile velocity differs by 4%, a larger difference than noted in the JA2 simulation.

Table 5. Comparison of IBHVG2 and IBBLAKE for Simulation of 120-mm Gun Using a HAN/Methanol/Water Mixture

	Maximum Pressure (MPa)	Muzzle Velocity (m/s)
IBHVG2	350	1,128
IBBLAKE	349	1,172

Thus, it appears that IB models using constant thermochemical values at a loading density of 0.2 g/cm^3, combined with pressure-dependent experimental data reduced at the same *ld*, provide good simulation of traditional solid propellant guns based on this limited study. However, ETC propellants combined with electrical energy may display thermochemical properties which are more strongly affected by loading density considerations. Thus, it appears that traditional IB methods of approximating the properties of the propelling gas may not be adequate in ETC simulations.

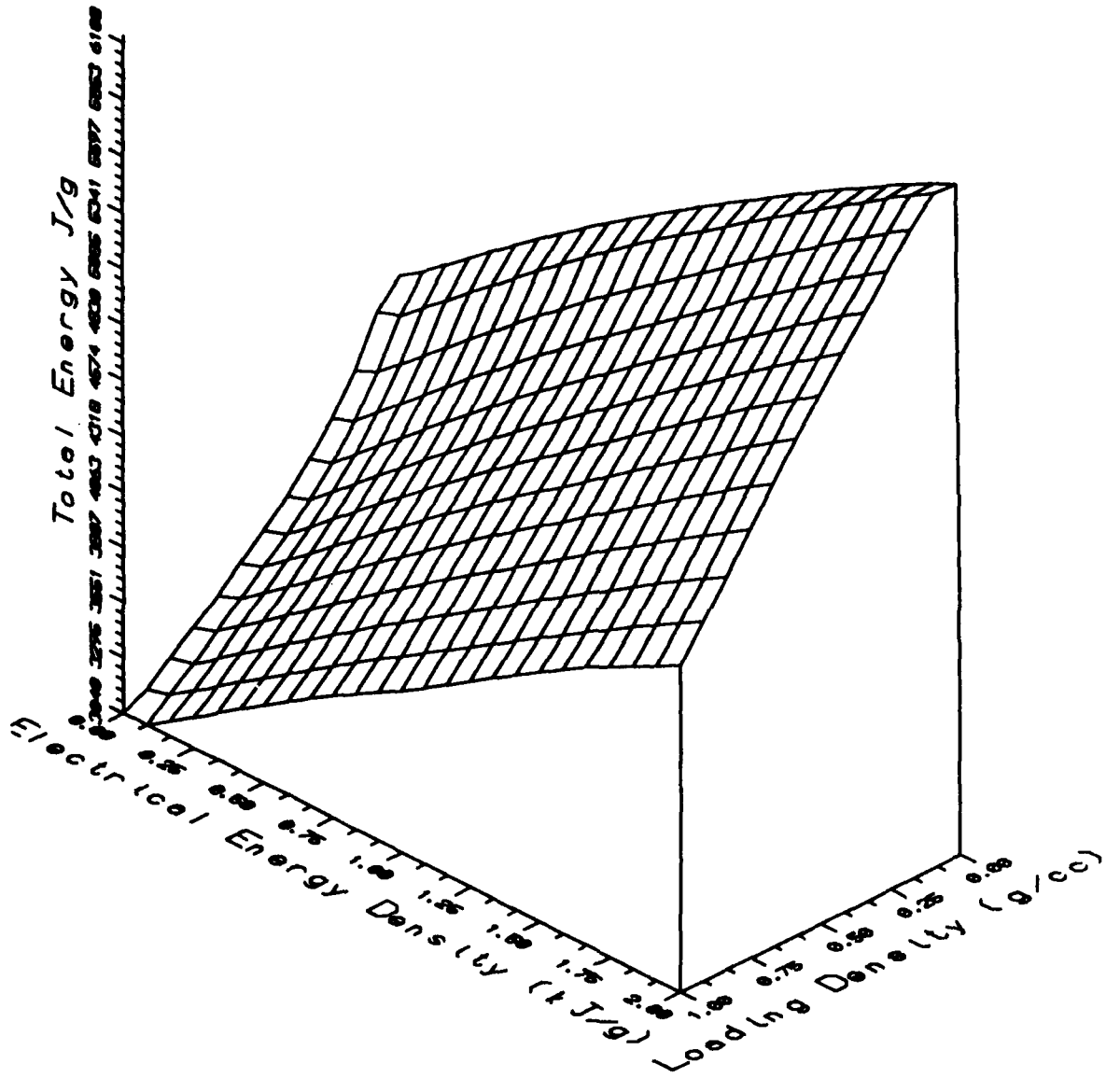


Figure 3. Energy vs. Loading Density vs. Electrical Energy Density for a Propellant 80% by Mass of HAN and Methanol in a Stoichiometric Mixture and 20% Water.

4. COMPARISON WITH INVERSE MODEL

An inverse model was developed previously (Wren and Oberle 1990, 1992) using variable thermochemistry at ld = 0.2 g/cm^3 and applied to a number of experimental shots. The model requires experimental breech pressure, projectile position, and electrical energy input at a time step and infers the mass of propellant consumed based on an energy balance equation. At gun pressures, compression of the liquid propellant can result in volume changes which affect the calculation of consumed mass. Thus, the model has been extended to treat compression of the working fluid (propellant) and consider losses as well as to extrapolate the thermochemical data (Wren and Oberle 1992). The model was revised for this study to permit the use of BLAKE as a subroutine. The mass of propellant consumed is that required to produce the space-mean pressure inferred from the experiment.

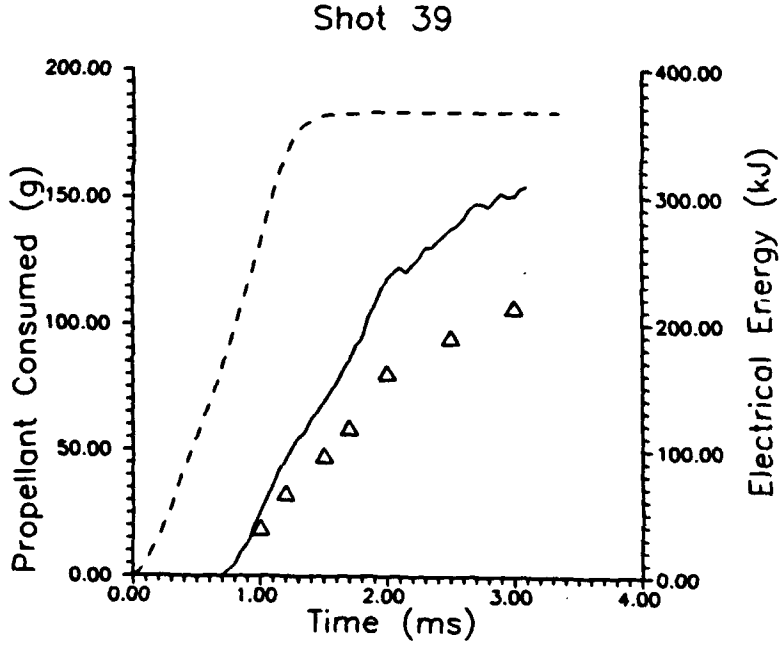
Electrical energy input for a 30-mm experimental firing, Shot 39, performed by GT-Devices (Greig 1990) as part of a repeatability series using titanium hydride and water is shown in Figure 4 by the dotted line. The previous inverse model results (Wren and Oberle 1992) using a table of variable thermochemical properties (see Table 6) at a fixed ld of 0.2 g/cm^3 is shown in Figure 4 by the solid line. In previous work, thermochemical values outside the range of Table 6 were taken to be the first and last values in the table (Wren and Oberle 1990) or were extrapolated (Wren and Oberle 1992). However, early (during the first millisecond) in the IB cycle, electrical energy densities are predicted to be quite high (above 10 kJ/g) and temperatures are high (above 5,000 K). However, the projectile motion is also not well described during the first millisecond in Shot 39. Hence, the estimate of mass consumed during the time from 0.0 to 1.0 ms is not reliable. It is noted that the inverse analysis is an energy balance at each time step independent of any other time step. Hence, the difficulty with prediction of mass consumed from 0.0 to 1.0 ms does not influence the prediction at a later time. The total mass of propellant in the experiment is 168.84 g. As indicated by the solid line in Figure 4, approximately 150 g of propellant is inferred to be consumed using a variable thermochemistry table (Table 6).

The linked inverse-BLAKE code (INVBLAK) results are shown by the triangles in Figure 4. It is seen that significantly less fluid is inferred to be consumed. These results are consistent with experimental observations that a quantity of unburned fluid was present at the conclusion of these shots (Greig 1990). For comparison, the ld vs. time required by BLAKE to match the experimental space-mean pressure is shown in Figure 5. It is noted that the ld stays below 0.1 g/cm^3, a regime in which the specific energy is higher than for a ld of 0.2 g/cm^3 (see Figure 3). The experiment has a large amount of ullage initially,

and if all the propellant reacted, the final *ld* would be 0.07 g/cm^3. Thus, the inclusion of thermochemical dependence on loading and electrical energy densities in the inverse model appears to provide a better estimate of the mass of propellant consumed in the ETC gun firing examined.

Table 6. Variable Thermochemical Values for 50% Ti_3H_2 and 50% H_2O Plus Electrical Energy at *ld* = 0.2 g/cm^3

Electrical Energy Input (kJ/g)	Temperature (K)	Impetus (J/g)	Molecular Weight	γ	Specific Energy (J/g)
2	2,162	679.3	6.716	1.2722	2,500
3	2,630	826.7	6.714	1.2722	3,240
4	3,078	969.0	6.704	1.2553	3,970
5	3,502	1,106.3	6.682	1.2443	4,670
6	3,899	1,239.2	6.645	1.2370	5,330
7	4,265	1,368.6	6.596	1.2325	5,950
8	4,604	1,495.8	6.546	1.2302	6,520
9	4,917	1,622.4	6.506	1.2294	7,060
10	5,210	1,749.4	6.487	1.2313	7,560



Note: Experiment electrical energy input (dotted). Mass of propellant consumed based on inverse model with table of thermochemical values (solid). Mass of propellant consumed based on inverse model linked to BLAKE (triangles).

Figure 4. Inverse model results for 30-mm titanium hydride and water firing.

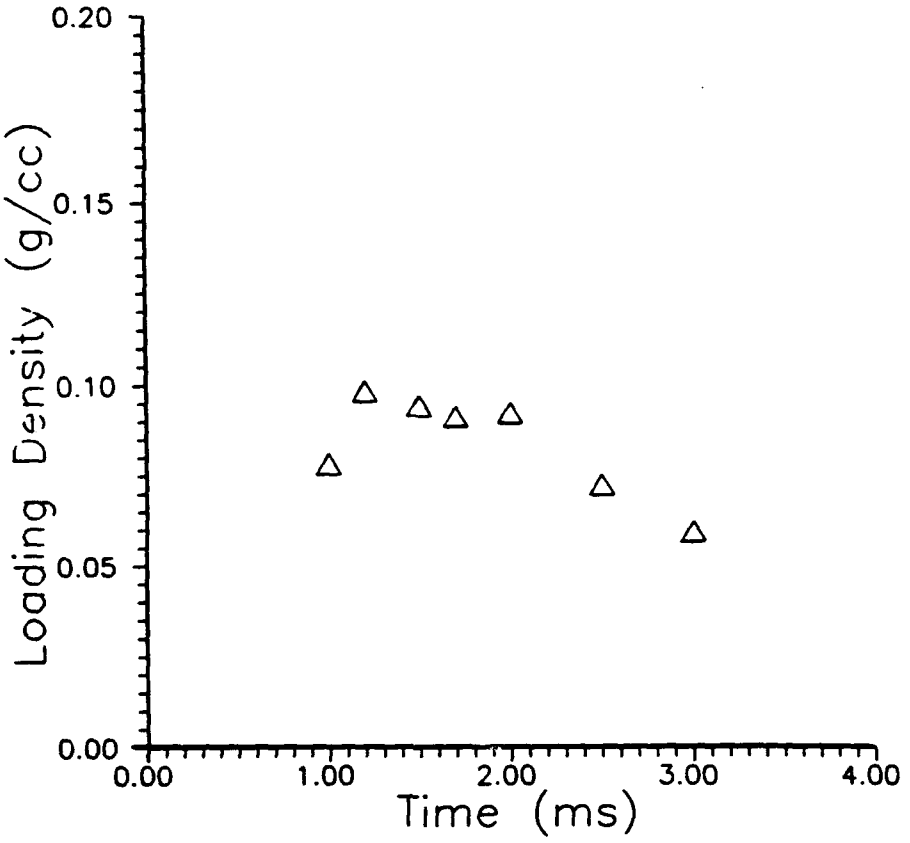


Figure 5. Loading density vs. time for 30-mm titanium hydride and water firing based on inverse model linked to BLAKE.

5. CONCLUSIONS

A thermochemical equilibrium code, BLAKE, has been directly linked to both an IB code and an inverse code in order to assess the potential improvement in describing the energy release rate in ETC gun modeling. The inverse analysis attempts to determine the decomposition or gas generation rate necessary to satisfy an energy balance equation based on experimental data.

The analysis was applied to the following: 1) a simulation of a standard 120-mm gun with JA2 propellant; 2) a simulation of a standard 120-mm gun with a potential representative ETC propellant; and 3) an inverse model of a 30-mm experimental firing using titanium hydride and water as the propellant (working fluid). The results suggest the following:

(1) The thermochemical code BLAKE can function as a subroutine to an IB code.

(2) Constant values of thermochemical properties and burn rates used in solid propellant modeling yield comparable results to the linked thermochemical-IB model.

(3) There is a greater difference between an IB simulation linked to BLAKE of an ETC propellant and an IB simulation using constant thermochemical values than with traditional solid propellants. The muzzle velocities differ by 4%, a larger difference than the solid propellant considered.

(4) A consideration of variable thermochemistry via a direct link to BLAKE in an inverse model (as opposed to tables of thermochemical values based on a constant loading density of 0.2 g/cm^3) makes a significant difference in the inferred values of mass of propellant consumed.

(5) Treatment of the dependence of thermochemistry on both electrical energy density and loading density appears to provide a better model of the state of the propelling gas in ETC applications.

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